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CFD Modeling of N_2/H_2 gaseous flow with geometric variations in a monolithic channel

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Abstract

Geometric variations by means of orientation of obstructions to the fluid flow can have a significant effect on the flow dynamics of gases in pursuit of maintaining required mixing in a low Reynolds number flow for a prospective reaction between the two gases. In this study, the effect of placing the obstructions parallel and perpendicular to the N_2 and H_2 flow was observed initially. Parallel placement resulted in favorable conditions in maintaining the desired ratio of the two components giving more than 90% mixing index throughout the channel length while perpendicular placement signaled better lateral movement on encountering the obstruction. Taking a cue from this, geometries having a combination of parallel and perpendicular obstructions were proposed based on results of parametric study on number of wires and spacing between them. Increasing perpendicular obstruction sets beyond 5 took the mixing index down to as low as 60 %. Increasing spacing from 1.5 mm to 2 mm deteriorated mixing index further but reducing perpendicular sets from 5 to 3 with 2 mm spacing resulted in 90 % mixing index throughout the channel and benchmark observed in axial-only configuration was regained. Also, increasing number of axial wires on a given perpendicular set or reducing their spacing did not alter desired mixing index to a great extent.

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*Keywords:*CFD, Nitrogen, Hydrogen, Flow Dynamics, Obstruction Orientation

1. Introduction

There has been a paradigm shift in the way essential chemicals are to be manufactured in the future. Growing concerns in regard with the energy and space requirements have elicited a lookout for the alternatives. Microchannels have surfaced to be suitable replacement to the present reactors on account of better heat transfer, smaller space requirement, higher interfacial area of contact, provision of safe environment for toxic chemicals because of lower amount used, and ease of integration into higher capacity production [1-3].

In view of high energy consumption and employment of high temperature and pressure conditions by Haber Bosch process, an alternative route for NH_3 manufacture was suggested using the alteration of electromagnetic properties of the reactants and

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conducting the reaction in microfluidic environment at ambient state. NH_3 synthesis through the mentioned route has been successfully proven at laboratory scale by Yahya et.al. [4].

Microchannels have a great potential to serve as reactors and heat exchangers after some improvement in certain areas. Mixing is one such area that poses a challenge to the wider applicability of microchannels, particularly when fast chemical reactions are involved. Because of smaller size, lower flow rate is required which creates problems in inducing mixing, especially lateral mixing. Given this constraint, mixing can be induced in a given geometry size and flow conditions through chaotic advection by placing obstructions to the flow [5]. This comes under passive mixing scheme which employs flow energy to promote mixing by means of lamination, chaotic advection, and inducing turbulence by specialty flow configurations. Passive micromixers are more popular on account of simplicity in construction [6]. The broad aim of a mixing scheme involving modifications to the geometry is to increase interfacial contact between the two fluids and to reduce the diffusion length [7].

Several micromixer designs for straight channels having obstructions to the flow have been proposed previously inflicting splits and recombination to path main flow [8] employing J shaped vessels [9], cylindrical obstructions [5], and diamond shaped obstructions [10]. Further geometric variations employed include patterned groove micromixer [11], convergent-divergent channel walls with circular variations [12], convergent-divergent channel walls with sinusoidal variations [13], cylindrical obstructions within curved microchannels [8], 3D Tesla structure [14] and diverging microchannel [15].

This CFD study intends to analyze the effect of obstructions on the dynamics of N_2/H_2 flow in a channel keeping in view that these obstructions would be utilized as flow inhibitors cum catalyst sites for prospective reaction. The obstructions in purview of this study are circular wires. The effect of the axial as well as perpendicular orientation of the obstruction with respect to the flow direction has been studied. This arrangement renders this geometry similar to a monolithic structure as a result of which 'monolithic' term has been used. The scope of this study does not consider effect of reaction and magnetic field. With NH_3 being synthesized successfully at smaller scale at ambient conditions, it is expected that increasing the number of wires (catalyst surface area) and placing them in right orientation would help improve yield.

Nomenclature

X_i	Mole Fraction at point/node i
$\overline{X}$	Optimal Mixing Fraction
σ^2	Actual Variance
σ^2_{max}	Maximum Possible Variance from Optimal Mixing Fraction
MI	Mixing Index
N	No. of sampling points

2. Methodology

The investigation protocol in this study includes qualitative analysis from streamlines and volume fraction contours along with quantitative analysis from a variance based index [8, 16, 17]. Streamlines give an idea of the path followed while volume fraction contours represent the volume/molar ratio with the mole fraction data utilized in the mixing index.

ANSYS CFX 15.0 [18] has been used for analysis which solves Navier-Stokes equations using finite volume approach for individual components. K-epsilon turbulence model has been used for Reynolds averaging of Navier-Stokes equations. Inlet velocity of 0.05 m/sec has been used for the gases which are introduced into the channel at the inlet in 1:3 ratio. ANSYS Meshing was used for meshing and acceptable mesh quality was ensured. For walls, no-slip boundary condition was used with a constant inlet velocity being assigned to the inlet and a zero static pressure was specified at the outlet.

This numerical technique gives data at all the points in the domain for the parameters which include velocity, volume fraction, temperature, turbulence eddy dissipation and turbulence kinetic energy. Out of these, velocity (for plotting streamlines) and volume fraction would find use for the analysis in this scope of study.

The mixing index used to gauge the proximity of the flow ratio of two components with the desired one has been given below:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{n}(X_i - \overline{X})^2} \tag{1}$$

$$MI = 1 - \sqrt{\frac{\sigma^2}{\sigma^2_{\max}}} \tag{2}$$

The optimal mixing fraction is considered as 0.75 mole fraction for hydrogen gas and 0.25 mole fraction for nitrogen gas. This is the point when the mixture would be in the desired 1:3 nitrogen to hydrogen ratio. The channel size is 10 mm x 50 mm with 3mm distance given at the entry for premixing before it encounters the obstructions. Multiple variations of obstruction placement have been analyzed based on the parameters covering orientation, number of obstructions, and spacing.

The first set of analysis was aimed at observing principal difference between flow with obstructions parallel or perpendicular to it. In that pursuit, two geometries were chosen with one having a set of wires placed parallel and another having set of wires placed perpendicular to the fluid flow with detailed dimensions shown in Fig. 1. Based on these observations, the geometries with a combination of parallel as well as perpendicular obstructions were proposed (Fig. 2) and fluid flow was analyzed as per the protocol defined.

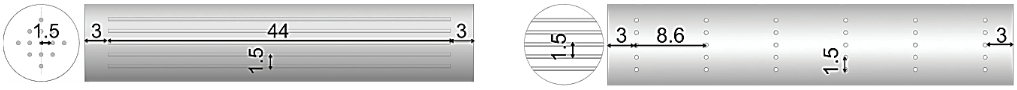
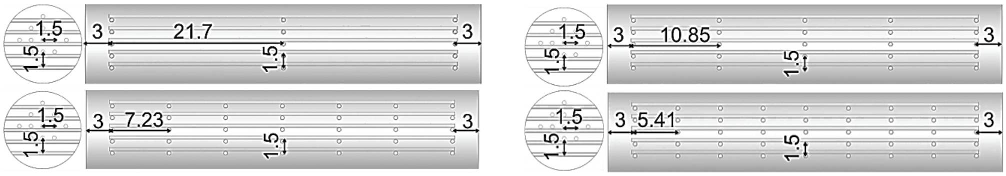
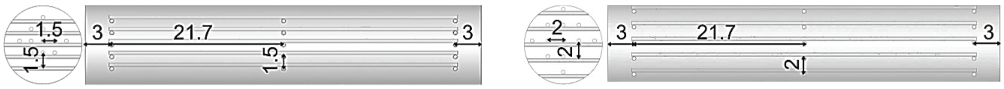


Fig. 1 The geometries considered for comparative analysis of flow for parallel or perpendicular obstructions to the flow.



(a)



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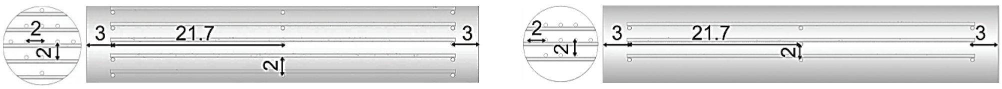

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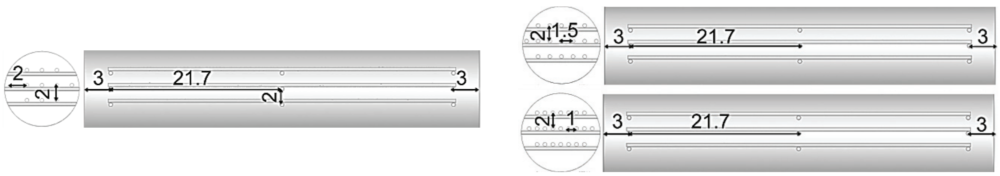


(d)

Fig. 2 Schematic diagram of channel for: a) Flow with same pattern of axial wires and increasing the perpendicular support sets axially, b) Flow with increasing the spacing between wires c) Flow with radially decreasing the number of wires in a perpendicular set of supports, d) Flow with increasing the number of axial wires placed on a given perpendicular support. All the dimensions are in mm.

3. Results and Discussion

3.1. Comparison between axial and perpendicular orientation of obstructions

For the first set of analysis, one of the geometry contained 13 wires arranged axially and another contained set of 30 wires arranged perpendicular to the flow which was of varied sizes in accordance with the chord dimensions they are placed into (Fig. 1).

As shown in Fig. 3, for flow having axial obstructions, the volume fraction did not alter to a great extent from the desired one (0.75 H_2 volume fraction represented in the volume fraction contours by yellow color) presenting a favorable outcome in terms of mixing index but streamlines presented a straight path. For flow having perpendicular obstructions, the mixing index was lesser than that of the one having axial obstructions but there is lateral movement on encountering obstructions which gives advantage to this setup as lateral movement in the bulk flow would affect movement in the constituting molecules and would result in enhanced collisions. A comparison of the extent of lateral movement in both the setups has been presented in Fig 4. Comparison based on the mixing index has been presented in Fig. 5.

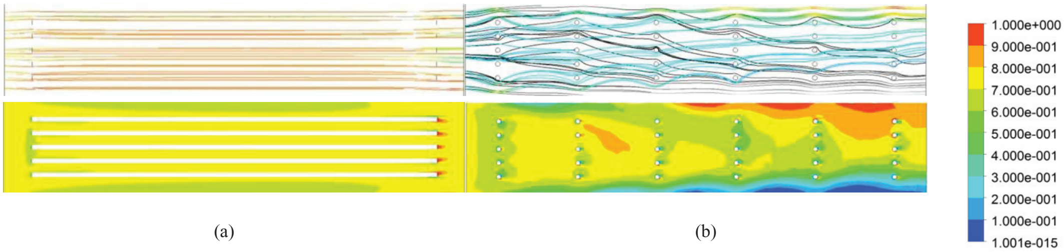


Fig. 3 Comparison of streamlines and volume fraction contours for a) axial and b) perpendicular placement of wires at the center of YZ axis. Colored Streamlines: Hydrogen flow, Grayscale streamlines: Nitrogen flow

Analyzing with another point of view, the perpendicular obstruction offer almost half the area of wire for contact as gas would approach from one end only. Further, the surface area available with the perpendicular wires (1601 mm^2 as compared with 11681 mm^2 for axial wires for geometries considered) is also very less.

This leaves us with the option to have combined axial as well as perpendicular set of obstructions. The axial set holds the edge in terms of uninterrupted catalyst site option throughout the channel with the whole area to offer for gas interaction. Perpendicular obstructions, by virtue of providing bumps to the flow at regular intervals result in enhanced lateral interaction leading to better mixing. This led us to the next set of analysis which involves the parametric study for this pattern of obstruction placement gradually heading to better geometries.

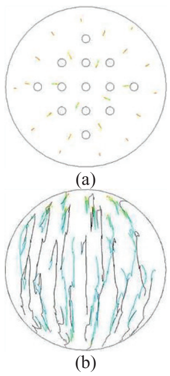


Fig. 4 Comparison of streamlines of a) axial and b) perpendicular placement of wires viewed from XY axis as reference

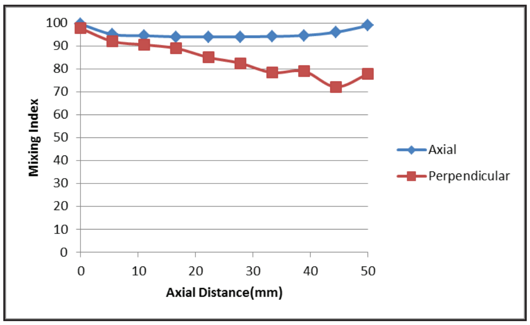


Fig. 5 Variation of desired mixing ratio represented through mixing index (For section 3.1)

3.2. Analysis of effect of number of obstructions and spacing between them

3.2.1. Effect of increasing perpendicular support sets for the same number of axial orientation wires

Increasing the perpendicular obstructions provided more number of bumps to the flow (Fig. 6). However, increasing the number of obstructions to a certain extent (From 3 to 5) has resulted in better mixing dynamics but it began deteriorating on further increasing the obstructions (to 7 and 9 respectively) as shown graphically in Fig. 7. In case of increased obstructions there is greater space with excessive hydrogen fraction (represented by red region) as shown in Fig. 6(c) and Fig. 6(d). Also, there is significant presence of red region in between subsequent sets of perpendicular obstructions in this section having 1.5 mm spacing.

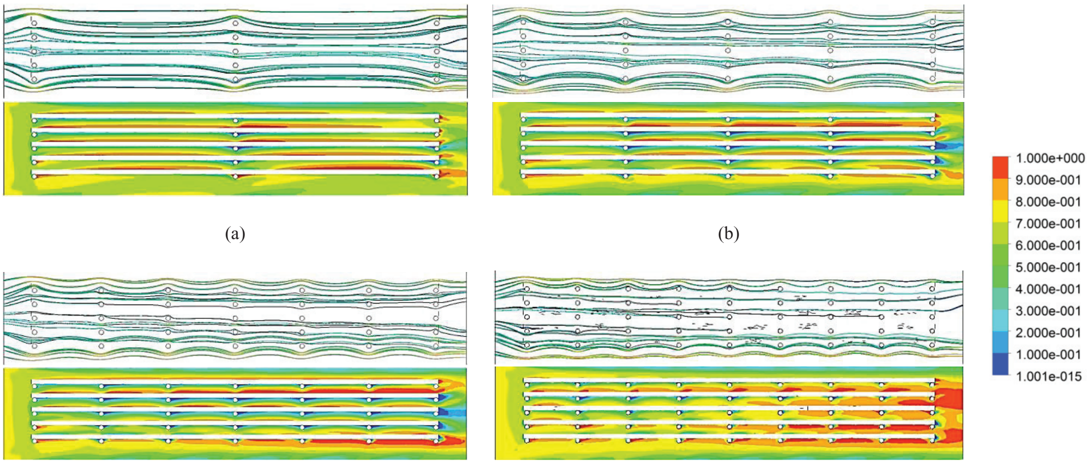


Fig. 6 Volume fraction contours and streamlines at center of YZ axis of geometries selected for analysis on a) 3 sets, b) 5 sets, c) 7 sets, and d) 9 sets of perpendicular obstructions keeping the same pattern of axial obstructions (13 wires). Colored Streamlines: Hydrogen flow, Grayscale streamlines: Nitrogen flow

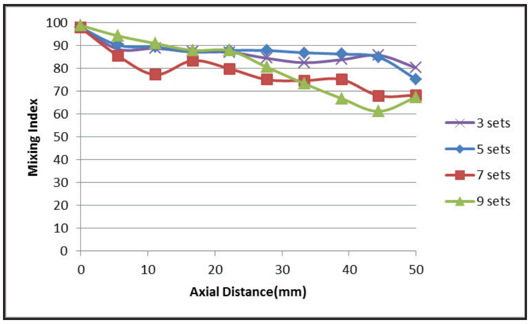


Fig. 7 Variation of desired mixing ratio represented through mixing index (For section 3.2.1)

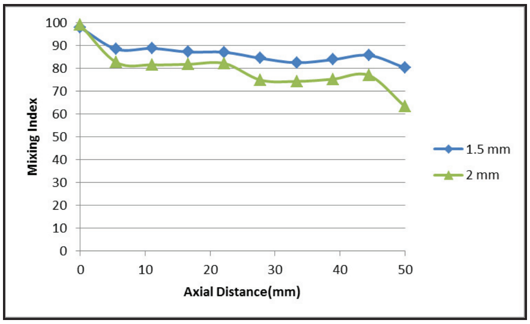


Fig. 8 Effect of increasing radial spacing between perpendicular sets on mixing index (For section 3.2.2)

3.2.2. Effect of radial spacing between subsequent perpendicular obstruction sets keeping axial pattern constant

Increasing the spacing between the perpendicular wires from 1.5 mm to 2 mm was carried out in view of obtaining better dynamics, particularly in the region between the subsequent wires. This, however, has resulted in decreased mixing index to as low as 70% for major part and 60% towards the end as shown in Fig. 8. On increasing spacing, the topmost and bottommost set comes very close to the wall and it becomes difficult for the comparatively heavier nitrogen gas to keep up with the pace of the hydrogen gas in that region. Hence, this region is primarily occupied by hydrogen gas (Fig. 9) resulting in inferior mixing dynamics. Streamlines also present a comparatively straighter path. However, there is lesser proportion of red region in between the wires in the central region signaling a better prospect.

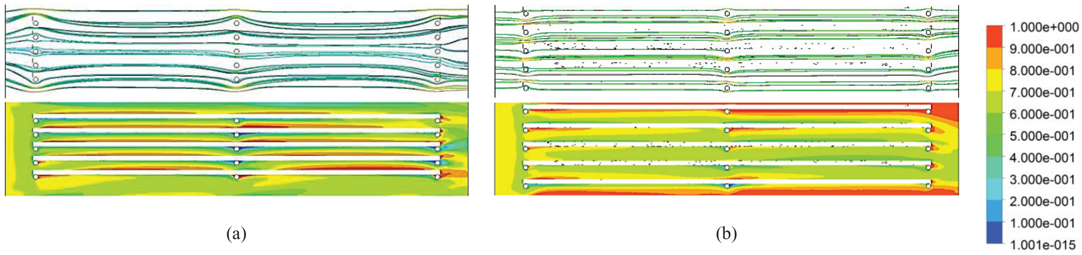


Fig. 9 Volume fraction contours and streamlines at center of YZ axis of geometries selected for analysis by varying the spacing by a) 1.5 mm to b) 2 mm between wires in a given perpendicular set. Colored Streamlines: Hydrogen flow, Grayscale streamlines: Nitrogen flow

3.2.3. Effect of number of wires (or supports) in the perpendicular set of obstructions

Reducing the number of wires in a given perpendicular obstruction set was considered for improving dynamics in case of increased spacing. Removing a set from the top and the bottom has presented better results as shown in Fig. 10. Using 3 sets of obstructions has kept the mixing above 90% throughout (Fig. 11) and hence, it would not be desirable to reduce the set of obstructions further and explore the possibility of increasing the number of axial wires and, in turn, the catalyst surface area within this arrangement. This reduced perpendicular set arrangement has also given much broader yellow region as compared to the one with 5 sets and the ones observed in the section with 1.5 mm spacing.

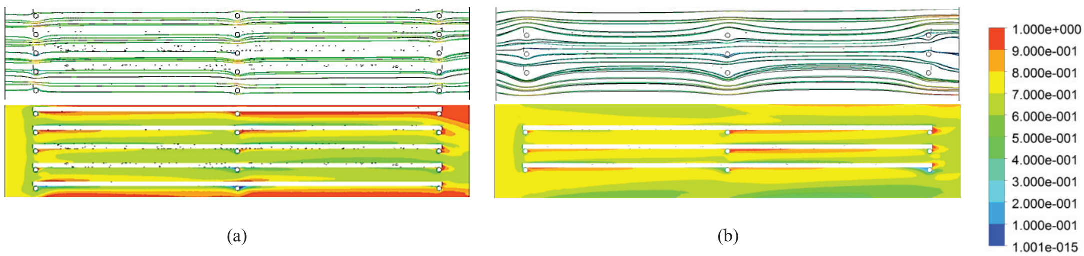


Fig. 10 Volume fraction contours and streamlines at center of YZ axis for geometries selected for analysis having a) 5 wires and b) 3 wires in a given perpendicular obstruction set respectively. Colored Streamlines: Hydrogen flow, Grayscale streamlines: Nitrogen flow

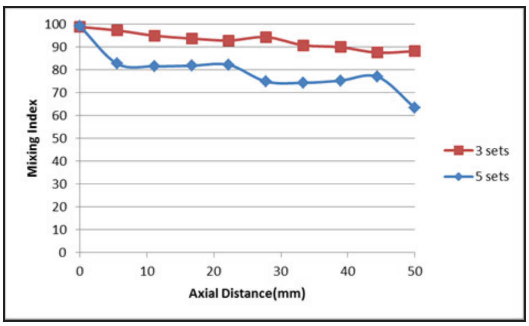


Fig. 11 Variation of mixing index on reducing number of supports in 2 mm spacing (For section 3.2.3)

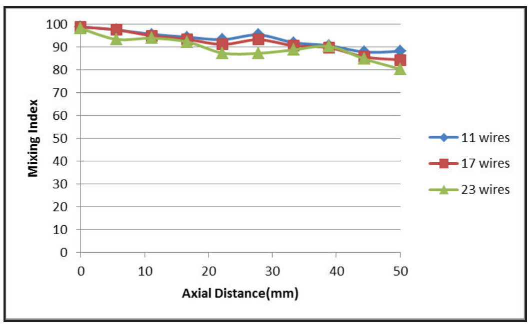
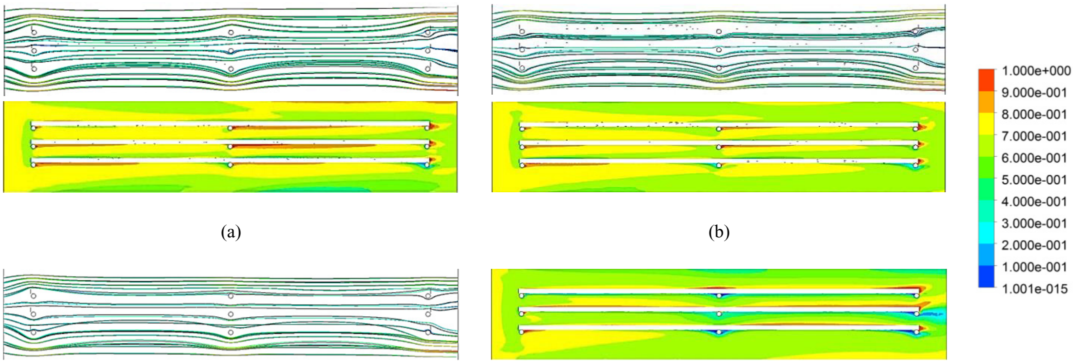


Fig. 12 Variation of desired mixing ratio represented through mixing index (For section 3.2.4)

3.2.4 Effect of increasing the number of axial wires on a given perpendicular support

Increasing the number of wires on a given perpendicular set does not affect the mixing index to a great extent even though it required reducing the axial spacing (Fig. 2(d)) between them. Mixing Index variation is shown graphically in Fig. 12 which suggests maintenance of close to 90 % mixing index throughout the channel. Streamlines suggest significant bumps on encountering the obstructions (Fig. 13). The desirable yellow region is maintained for a major part in first two geometries and the highly undesirable red region is virtually non-existent in all the geometries under consideration suggesting that there is no considerable disturbance in mixing profile on increasing the number and changing the spacing in obstructions placed axial to the flow.



(c)

Fig. 13 Volume fraction contours and streamlines for geometries selected for analysis with a) 11 wires (2 mm spacing), b) 17 wires (1.5 mm spacing) and c) 23 wires (1 mm spacing) arranged axially over same perpendicular obstruction set

4. **Conclusion**

In the first set of analysis, the principal difference between axial and perpendicular orientation of obstructions was analyzed. Axial orientation did not alter the mixing index to a great extent, thereby, maintaining the desired ratio between the two components. However, streamlines suggest that gases followed straight path with minimal lateral movement. Inducing lateral movement which is expected to enhance collisions was achieved by placing wires perpendicular to the flow. Axial wires ensured surface for the catalyst site throughout the channel while perpendicular wires were a necessity as they serve as support to hold the axial wires along with providing the lateral mixing by employing bumps to the flow. Increasing the perpendicular set of wires beyond a certain extent (5 wires) deflects the mixing index from the desired ratio as the comparatively heavier Nitrogen gas does not keep up with the pace of Hydrogen gas. Increasing the spacing from 1.5 mm to 2 mm was also studied with aim of improving the dynamics, particularly in the region in vicinity of wires and facilitating the ease of fabrication. Increasing the spacing in this setup, however, resulted in lower overall mixing index. The topmost and bottommost supports were closer to the wall and were blocking the Nitrogen flow in that area. The positive prospect from this set was the minimal presence of red region (which indicate lowest mixing dynamics) in the central core in comparison with previously observed geometries. Following this observation, the topmost and bottommost sets were removed with aim of improving overall mixing dynamics. This arrangement almost eradicated the red region from the channel, regained the mixing index of 90% throughout the channel and achieved benchmark observed initially in the axial-only arrangement. This axial-perpendicular arrangement maintaining the same mixing index, offers advantage in terms of lateral interaction and fabrication. In view of maximizing the surface area for the catalyst site increasing the number of axial wires on a given perpendicular support was considered. This arrangement did not deteriorate the desired mixing index even in the case of decreased spacing between the wires to accommodate more wires. The number of wires and spacing in perpendicular sets had greater effect on mixing index as compared to quantity and spacing of wires in axial sets.

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